Methodology for determining the acceptability of system designs in uncertain environments

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Online Appendix of "Methodology for determining the acceptability of system designs in uncertain environments"

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1 Studentized prediction errors

The Studentized or normalized prediction errors are

$$z_{j;i} = \frac{q_{j;i} - \widehat{y}_{j;-i}}{\sqrt{\widehat{var(q_{j;i})} + \widehat{var(\widehat{y}_{j;-i})}}}. \tag{1}$$

The factor $\widehat{var(\widehat{y}_{j;-i})}$ in (1) follows from classic linear regression analysis:

$$\widehat{var(\widehat{y}_{j;-i})} = \mathbf{x}_i' \widehat{cov(\widehat{\boldsymbol{\beta}}_{j;-i})} \mathbf{x}_i$$

where

$$\widehat{cov(\widehat{\boldsymbol{\beta}}_{j;-i})} = (\mathbf{X}'_{-i}\mathbf{X}_{-i})^{-1}\mathbf{X}'_{-i}\widehat{\mathbf{cov}(\widehat{\mathbf{q}}^*_{j;-i})}\mathbf{X}_{-i}(\mathbf{X}'_{-i}\mathbf{X}_{-i})^{-1} \tag{2}$$

where $\widehat{\mathbf{cov}(\widehat{\mathbf{q}}^*_{j;-i})}$ results from eliminating row i and column i from the $n \times n$ matrix $\widehat{\mathbf{cov}(\widehat{\mathbf{q}}^*_j)}$ which has the elements

$$\widehat{cov(\widehat{q}^*_{j;i}, \widehat{q}^*_{j;i'})} = \frac{\sum_{b=1}^{B}(\widehat{q^*_{j;i;b}} - \overline{\widehat{q}^*_{j;i}})(\widehat{q^*_{j;i';b}} - \overline{\widehat{q}^*_{j;i'}})}{B-1}. \tag{3}$$

The factor $\widehat{var(q_{j;i})}$ in (1) is estimated through the bootstrapped estimator $\widehat{var(\widehat{q}^*_{j;i})}$, which follows from (3) in case $i = i'$.

Note: The correlation coefficients

$\rho_{j;i;i'} = \widehat{cov(\widehat{q}^*_{j;i}, \widehat{q}^*_{j;i'})} / \sqrt{\widehat{var(\widehat{q_{j;i}})}\widehat{var(\widehat{q_{j;i'}})}}$

quantify the effects of CRN. Furthermore, Kleijnen (2008, p. 61) uses the Student statistic with $m-1$ degrees of freedom t_{m-1} instead of standard Normal variable z, but we study a quantile instead of an average. Finally, we cannot use the shortcut in Kleijnen (2008, p.61)—which uses the so-called hat-matrix $\mathbf{H} = \mathbf{X}(\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'$—because that shortcut assumes white noise.

Because (1) gives n values for each product j ($j = 1,\ldots,s$), we reject the regression metamodel for product j if

$$\max_i |z_{j;i}| > z_{1-[\alpha/(2n)]} \tag{4}$$

where the right-hand side follows from *Bonferroni's inequality*, which implies that the classic type-I error rate (in this case $\alpha/2$ because the CI is two-sided) is replaced by the same value divided by the number of tests (namely, n).

In the example, we find that the test statistic $\max_{i;j} |z_{i;j}|$ defined in (4) is extremely significant, namely -192 in scenario 16 for product 1 and -1347 in scenario 7 for product 2. Our explanation is that the simulation outputs show very little variability, as we have already pointed out. This result illustrates that statistically significant results are not always important; see Kleijnen (2008, p.31) for a general discussion. In our case the normalized prediction errors are very significant, but the AREs are acceptable for our purpose, namely validating first-order polynomials and identifying the important factors in these polynomials. (Nevertheless, the test in (4) may be useful in other simulation models with more variability, so we do present this test—albeit in an appendix.)

2 Estimated variances of bootstrapped quantiles

Table 1 shows that $\max_i(\widehat{var(\widehat{q^*_{i;1}})})/\min_i(\widehat{var(\widehat{q^*_{i;1}})}) = 7.739/1.233 = 6.3$, whereas the ratio of the ranges of the distribution-free CIs was 7.5; see the main text. Product 2 gives $\max_i(\widehat{var(\widehat{q^*_{i;2}})})/\min_i(\widehat{var(\widehat{q^*_{i;2}})}) = 5.312/1.659 = 3.2$, whereas the distribution-free CIs gives 5.

3 Validation: scatterplots and cross-validation

Figures 1 and 2 give the scatterplots for products 1 and 2 respectively. Table 2 gives the first eight estimated effects for product 1 when applying cross-validation; Table 3 gives the remaining effects plus the estimated quantiles and AREs. Tables 4 and 5 give the analogous results for product 2. Figures 3 and 4 give scatterplots based on cross-validation.

Scenario	$\widehat{var}(\widehat{q^*_{i;1}})$	$\widehat{var}(\widehat{q^*_{i;2}})$
1	3.626	2.945
2	1.834	3.019
3	3.393	2.510
4	1.986	5.312
5	1.516	2.218
6	2.185	4.046
7	1.947	1.659
8	2.466	4.159
9	4.306	3.863
10	2.959	4.602
11	7.739	2.307
12	4.701	2.972
13	2.606	3.340
14	2.960	3.885
15	1.233	2.927
16	2.255	2.927

Table 1: Scenarios with bootstrapped variances of estimated outputs

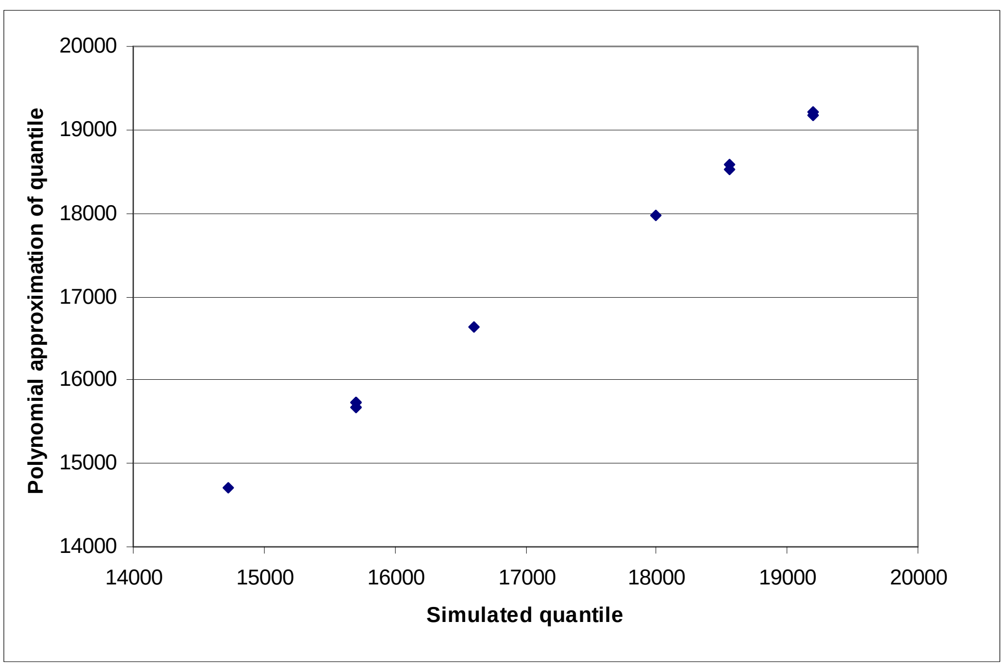

Figure 1: Quantiles simulated versus quantiles predicted through first-order polynomial for product 1

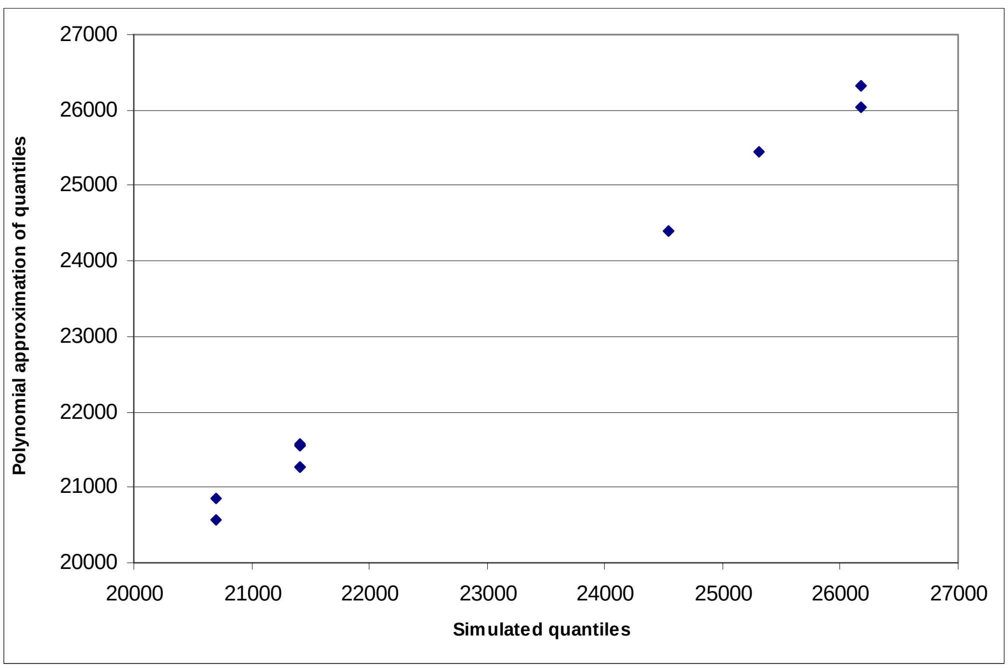

Figure 2: Quantiles simulated versus quantiles predicted through first-order polynomial for product 2

$-i$	$\widehat{\beta_{0;1}}$	$\widehat{\beta_{1;1}}$	$\widehat{\beta_{2;1}}$	$\widehat{\beta_{3;1}}$	$\widehat{\beta_{4;1}}$	$\widehat{\beta_{5;1}}$	$\widehat{\beta_{6;1}}$	$\widehat{\beta_{7;1}}$
0	17072.50	175.38	−24.75	−1490.00	297.75	−227.38	−297.88	−95.38
1	17097.63	200.50	49.88	−1464.88	322.88	−202.25	−272.75	−70.25
2	17047.38	150.25	−0.38	−1515.13	322.88	−252.50	−323.00	−70.25
3	17047.38	150.25	−0.38	−1464.88	272.63	−252.50	−272.75	−120.50
4	17097.63	200.50	49.88	−1515.13	272.63	−202.25	−323.00	−120.50
5	17047.38	150.25	49.88	−1515.13	272.63	−202.25	−323.00	−120.50
6	17097.63	200.50	−0.38	−1464.88	272.63	−252.50	−272.75	−120.50
7	17097.63	200.50	−0.38	−1515.13	322.88	−252.50	−323.00	−70.25
8	17047.38	150.25	49.88	−1464.88	322.88	−202.25	−272.75	−70.25
9	17047.38	200.50	−0.38	−1515.13	272.63	−202.25	−272.75	−70.25
10	17097.63	150.25	49.88	−1464.88	272.63	−252.50	−323.00	−70.25
11	17097.63	150.25	49.88	−1515.13	322.88	−252.50	−272.75	−120.50
12	17047.38	200.50	−0.38	−1464.88	322.88	−202.25	−323.00	−120.50
13	17097.63	150.25	−0.38	−1464.88	322.88	−202.25	−323.00	−120.50
14	17047.38	200.50	49.88	−1515.13	322.88	−252.50	−272.75	−120.50
15	17047.33	200.50	49.88	−1464.88	272.63	−252.50	−323.00	−70.25
16	17097.63	150.25	−0.38	−1515.13	272.63	−202.25	−272.75	−70.25

Table 2: Cross-validation for product 1, Part 1 (intercept plus first seven factor effects)

$\widehat{\beta_{8;1}}$	$\widehat{\beta_{9;1}}$	$\widehat{\beta_{10;1}}$	$\widehat{\beta_{11;1}}$	$\widehat{\beta_{12;1}}$	$\widehat{\beta_{13;1}}$	$\widehat{\beta_{14;1}}$	$\widehat{q_{-i;1}}$	ARE
−147.75	54.00	−175.00	104.88	147.88	218.13	68.25		
−122.63	79.13	−149.88	130.00	173.00	243.25	93.38	16107	0.0255
−172.88	79.13	−149.88	79.75	173.00	243.25	93.38	14322	0.0273
−122.63	28.88	−149.88	130.00	122.75	243.25	93.38	18792	0.0209
−172.88	28.88	−149.88	79.75	122.75	243.25	93.38	18960	0.0216
−122.63	79.13	−200.13	130.00	173.00	193.00	93.38	15304	0.0255
−172.88	79.13	−200.13	79.75	173.00	193.00	93.38	16107	0.0256
−122.63	28.88	−200.13	130.00	122.75	193.00	93.38	19598	0.0209
−172.88	28.88	−200.13	79.75	122.75	193.00	93.38	18793	0.0209
−172.88	28.88	−200.13	130.00	173.00	243.25	43.13	15302	0.0256
−122.63	28.88	−200.13	79.75	173.00	243.25	43.13	16107	0.0255
−172.88	79.13	−200.13	130.00	122.75	243.25	43.13	19595	0.0209
−122.63	79.13	−200.13	79.75	122.75	243.25	43.13	17593	0.0223
−172.88	28.88	−149.88	130.00	173.00	193.00	43.13	16108	0.0255
−122.63	28.88	−149.88	79.75	173.00	193.00	43.13	15303	0.0255
−172.88	79.13	−149.88	130.00	122.75	193.00	43.13	18156	0.0216
−122.63	79.13	−149.88	79.75	122.75	193.00	43.13	17013	0.0242

Table 3: Cross-validation for product 1, Part 2

$-i$	$\widehat{\beta_{0;2}}$	$\widehat{\beta_{1;2}}$	$\widehat{\beta_{2;2}}$	$\widehat{\beta_{3;2}}$	$\widehat{\beta_{4;2}}$	$\widehat{\beta_{5;2}}$	$\widehat{\beta_{6;2}}$	$\widehat{\beta_{7;2}}$
0	23151.18	331.94	127.81	440.69	−1823.69	−440.94	−536.56	−243.19
1	23298.25	479.00	274.88	587.75	−1676.63	−293.88	−389.50	−96.13
2	23004.13	184.88	−19.25	293.63	−1676.63	−588.00	−683.63	−96.13
3	23004.13	184.88	−19.25	587.75	−1970.75	−588.00	−389.50	−390.25
4	23298.25	479.00	274.88	293.63	−1970.75	−293.88	−683.63	−390.25
5	23004.13	184.88	274.88	293.63	−1970.75	−293.88	−683.63	−390.25
6	23298.25	479.00	−19.25	587.75	−1970.75	−588.00	−389.50	−390.25
7	23298.25	479.00	−19.25	293.63	−1676.63	−588.00	−683.63	−96.13
8	23004.13	184.88	274.88	587.75	−1676.63	−293.88	−389.50	−96.13
9	23004.13	479.00	−19.25	293.63	−1970.75	−293.88	−389.50	−96.13
10	23298.25	184.88	274.88	587.75	−1970.75	−588.00	−683.63	−96.13
11	23298.25	184.88	274.88	293.63	−1676.63	−588.00	−389.50	−390.25
12	23004.13	479.00	−19.25	587.75	−1676.63	−293.88	−683.63	−390.25
13	23298.25	184.88	−19.25	587.75	−1676.63	−293.88	−683.63	−390.25
14	23004.13	479.00	274.88	293.63	−1676.63	−588.00	−389.50	−390.25
15	23004.13	479.00	274.88	587.75	−1970.75	−588.00	−683.63	−96.13
16	23298.25	184.88	−19.25	293.63	−1970.75	−293.88	−389.50	−96.13

Table 4: Cross-validation for product 2, Part 1

$\widehat{\beta_{8;2}}$	$\widehat{\beta_{9;2}}$	$\widehat{\beta_{10;2}}$	$\widehat{\beta_{11;2}}$	$\widehat{\beta_{12;2}}$	$\widehat{\beta_{13;2}}$	$\widehat{\beta_{14;2}}$	$\widehat{q_{-i;2}}$	ARE
−332.19	−39.06	−352.19	236.06	351.44	447.81	242.94		
−185.13	108.00	−205.13	383.13	498.50	594.88	390.00	23768	0.1098
−479.25	108.00	−205.13	89.00	498.50	594.88	390.00	22188	0.0958
−185.13	−186.13	−205.13	383.13	204.38	594.88	390.00	19063	0.1098
−479.25	−186.13	−205.13	89.00	204.38	594.88	390.00	27661	0.0929
−185.13	108.00	−499.25	383.13	498.50	300.75	390.00	19063	0.1098
−479.25	108.00	−499.25	89.00	498.50	300.75	390.00	28529	0.0898
−185.13	−186.13	−499.25	383.13	204.38	300.75	390.00	23770	0.1098
−479.25	−186.13	−499.25	89.00	204.38	300.75	390.00	23822	0.0898
−479.25	−186.13	−499.25	383.13	498.50	594.88	95.88	19063	0.1099
−185.13	−186.13	−499.25	89.00	498.50	594.88	95.88	28531	0.0898
−479.25	108.00	−499.25	383.13	204.38	594.88	95.88	23771	0.1098
−185.13	108.00	−499.25	89.00	204.38	594.88	95.88	22187	0.0958
−479.25	−186.13	−205.13	383.13	498.50	300.75	95.88	23769	0.1098
−185.13	−186.13	−205.13	89.00	498.50	300.75	95.88	23823	0.0898
−479.25	108.00	−205.13	383.13	204.38	300.75	95.88	18352	0.1136
−185.13	108.00	−205.13	89.00	204.38	300.75	95.88	23058	0.1136

Table 5: Cross-validation for product 2, Part 2 (last seven factor effects„ cross-validation, and ARE)

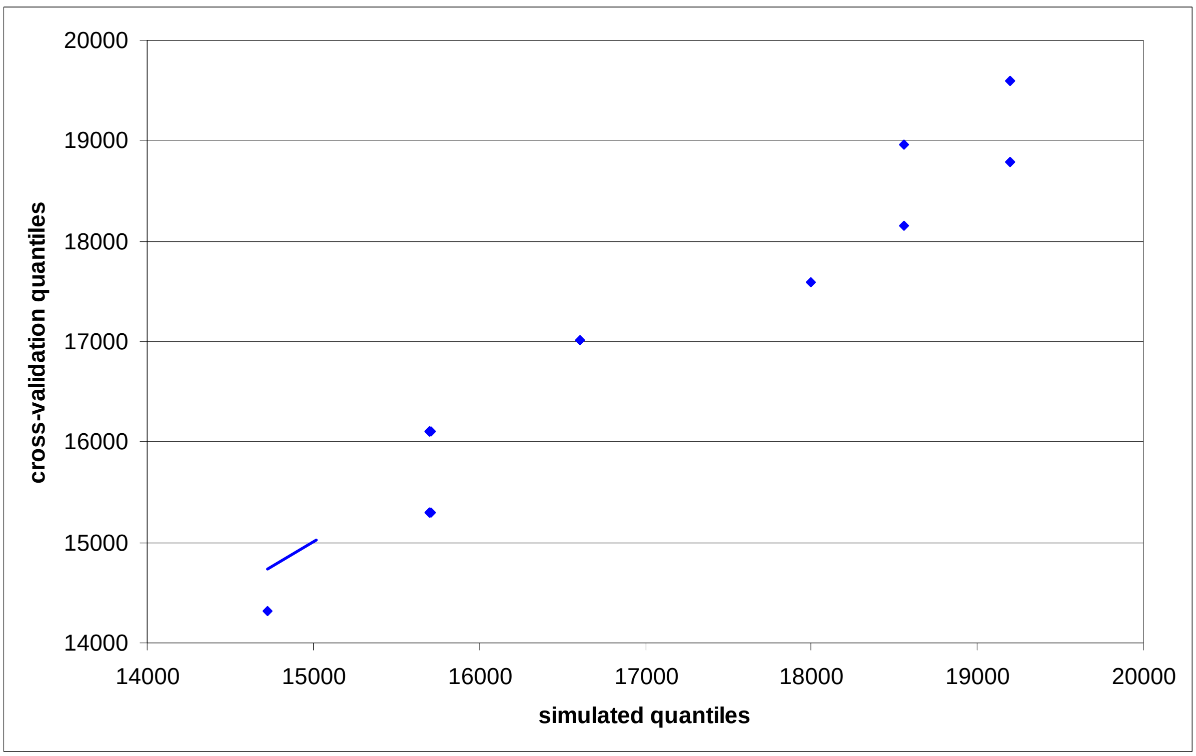

Figure 3: Scatterplot with simulated versus cross-validated quantiles for product1

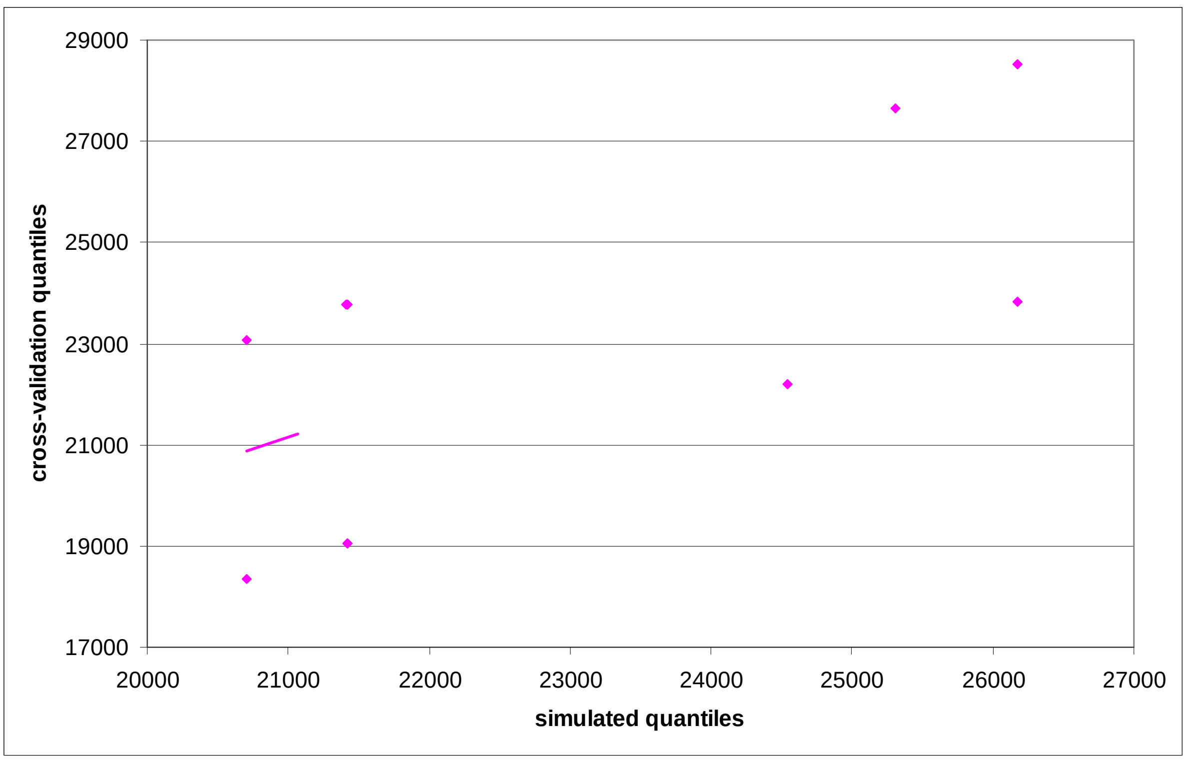

Figure 4: Scatterplot with simulated versus cross-validated quantiles for product 2

OLS estimate	$\widehat{\beta}^{*}_{(2.5);1}$	$\widehat{\beta}^{*}_{(97.5);1}$	$\widehat{\beta}^{*}_{(2.5);2}$	$\widehat{\beta}^{*}_{(97.5);2}$
0	17076.97	17083.50	23156.56	23162.81
1	174.13	175.31	331.94	332.31
2	25.06	26.13	127.31	127.81
3	−1491.06	−1490.56	440.63	441.31
4	297.81	298.25	−1824.44	−1823.66
5	−228.13	−227.50	−441.06	−440.63
6	−298.16	−297.81	−537.06	−536.50
7	−95.72	−95.31	−243.63	−243.13
8	−148.25	−147.81	−332.38	−331.94
9	54.56	55.63	−38.75	−38.50
10	−175.44	−175.00	−351.81	−351.50
11	104.69	105.63	235.94	236.44
12	147.75	148.06	351.75	352.13
13	218.13	218.38	447.63	448.19
14	68.00	68.31	243.13	243.44

Table 6: CIs for intercept and 14 factor effects, computed from 100 bootstrapped quantiles, for products 1 and 2

4 Bootstrapped confidence intervals for individual factor effects

Table 6 displays the 95% CIs for the individual factor effects, based on bootstrapping.

5 Graphically illustration of frontier

We illustrate the 14-dimensional frontier as follows. First we assume that all 14 parameters are at their base values; i.e., $\mathbf{x}' = (x_1, \ldots, x_{14}) = \mathbf{0}'_{14}$ where $\mathbf{0}_z$ denotes a vector with z zeroes. The estimated frontier then implies

$$E(\widehat{y_1} \mid \mathbf{x} = \mathbf{0}_{14}) = \widehat{\beta_{0;1}} \text{ and } E(\widehat{y_2} \mid \mathbf{x} = \mathbf{0}_{14}) = \widehat{\beta_{0;2}}. \tag{5}$$

Next we assume that a single parameter (say) x_h deviates from its base value while all other 13 parameters remain at their base values: $\mathbf{x}_{-h}= \mathbf{0}_{13}$. Then the estimated frontier implies

$$E(\widehat{y_1} \mid x_h, \mathbf{x}_{-h}= \mathbf{0}_{13}) = \widehat{\beta_{0;1}}+\widehat{\beta_{h;1}}x_h \text{ and } E(\widehat{y_2} \mid x_h, \mathbf{x}_{-h}= \mathbf{0}_{13}) = \widehat{\beta_{0;2}}+\widehat{\beta_{h;2}}x_h. \tag{6}$$

Then (5) and (6) give Figure 5 with the output $q_{j;0.05}$ as a first-order polynomial in the (coded) parameter x_h, assuming that $\widehat{\beta_{h;1}} > \widehat{\beta_{h;2}} >$

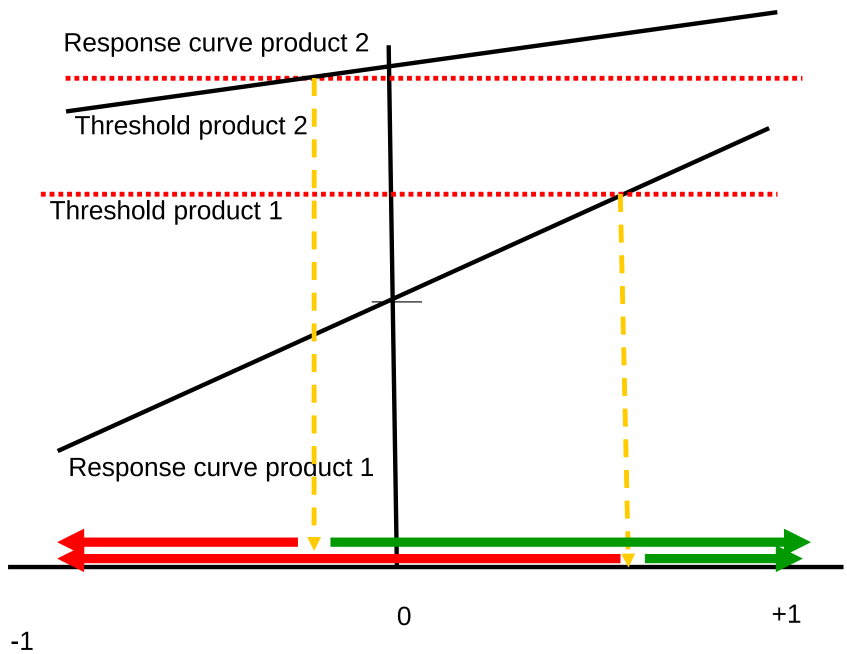

Figure 5: Acceptable and unacceptable factor variations

0. The two first-order polynomial response curves intersect (see dashed vertical lines) with the two corresponding thresholds (horizontal lines). These intersections give the acceptable ('green') variations and the unacceptable ('red') variations in x_h. Actually, the threshold for product 1 gives the truly acceptable variations, because product 2 gives a larger range of acceptable variations than product 1 but both thresholds must be satisfied.

Finally we assume that *two* parameters (say) x_h and $x_{h'}$ deviate from their base values while all other 12 parameters remain at their base values; we denote this scenario by $(x_h, x_{h'}, \mathbf{x}_{-(h;h')}= \mathbf{0}_{12})$. The estimated frontier then implies

$$\begin{aligned} E(\widehat{y_1} \mid x_h, x_{h'}, \mathbf{x}_{-(h;h')}= \mathbf{0}_{12}) &= \widehat{\beta_{0;1}} + \widehat{\beta_{h;1}} x_h + \widehat{\beta_{h';1}} x_{h'} \\ E(\widehat{y_2} \mid x_h, x_{h'}, \mathbf{x}_{-(h;h')}= \mathbf{0}_{12}) &= \widehat{\beta_{0;2}} + \widehat{\beta_{h;2}} x_h + \widehat{\beta_{h';2}} x'_h. \end{aligned} \tag{7}$$

To illustrate (7), we plot the effects of the two most important parameters for product 1—namely x_1 corresponding with the original parameter $\mu_{1;1}$ and x_2 or $\mu_{2;2}$ (see the main text)—and the threshold 15000:

$$14281.44 - 1063.31 x_1 + 180.6875 x_2 = 15000.$$

This equation gives Figure 6, which shows that low values for $\mu_{1;1}$ give acceptable production volumes. For product 2, all combinations of its

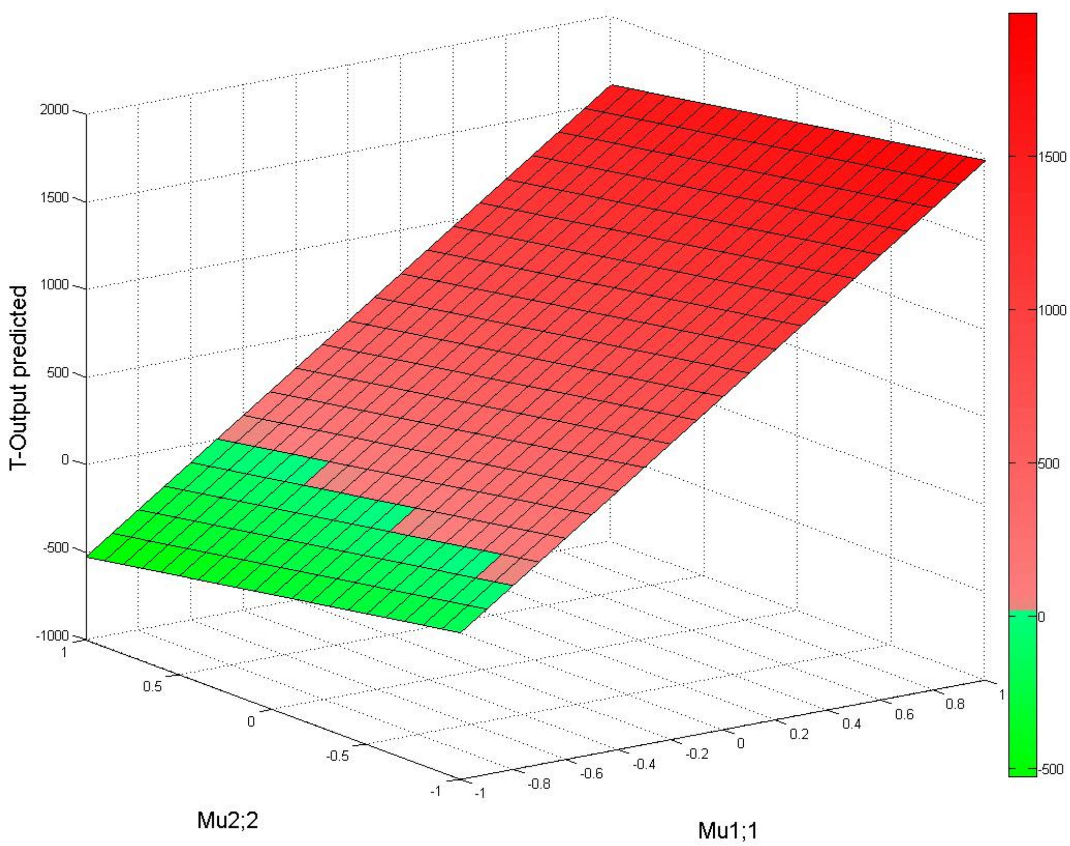

Figure 6: Acceptability frontier for product 1, when factors 1 and 2 change

two most important parameters—namely $\mu_{2;2}$ and $\mu_{2;3}$—give acceptable production volumes; we do not display this figure.

We point out that the acceptability of a change in x_h is also determined by the change in the other parameters $x_{h'}$—even though the estimated first-order polynomials imply that there are no parameter interactions. In practice, all parameters may deviate from their base values, so the two preceding figures are simplifications (meant to illustrate the issue); we recommend to use the analytical representation (see the main text) instead of the geometric representation.